A STUDY OF THE FORMAMIDE-$(H_2O)_3$ COMPLEX BY MICROWAVE SPECTROSCOPY

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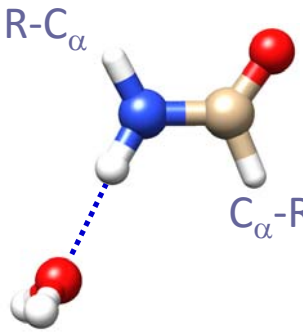
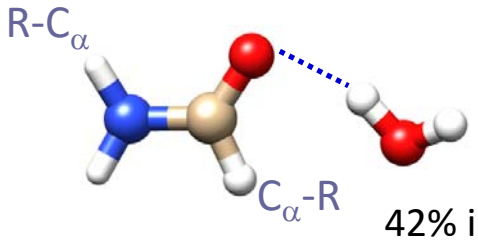
trans-peptide
~99%



FW-1:1c

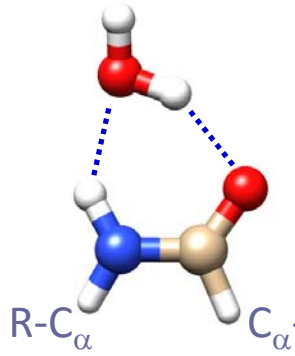
14% In proteins



FW-1:1b

42% in proteins

cis-peptide
~1%



FW-1:1a

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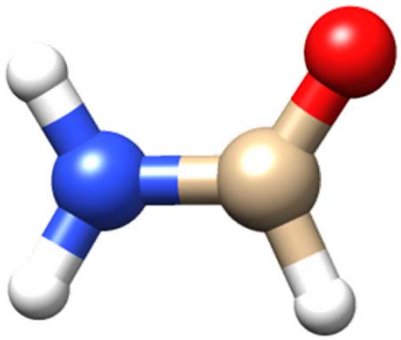
Interactions between peptide groups and water may be modelled from the study of gas phase **microsolvated** clusters of simple molecules such as **formamide**.



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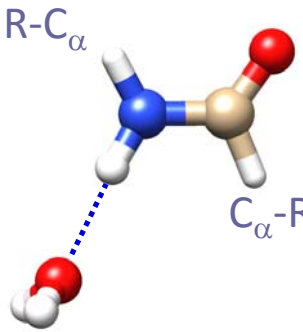
~99%



FW-1:1c

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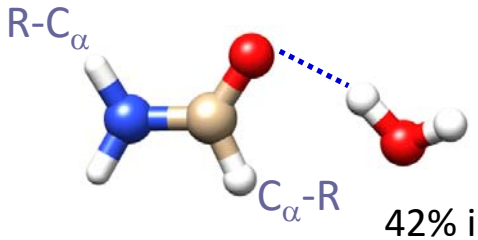

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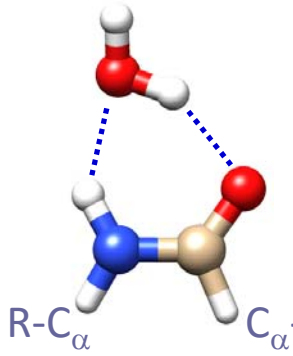
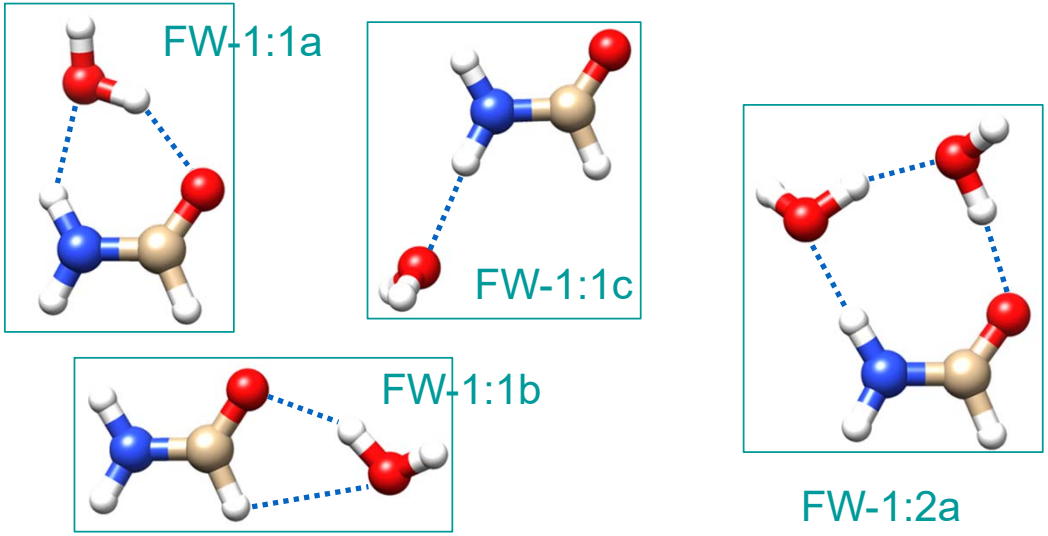


FW-1:1a

A STUDY OF THE FORMAMIDE-$(H_2O)_3$ COMPLEX BY MICROWAVE SPECTROSCOPY

We have analyzed the rotational spectra of formamide$_m$-$(H_2O)_n$ (m,n=1,2) clusters:

1) To characterize the different 1:1, 1:2, 2:1 conformers.



S. Blanco et al., *JACS 128(37) 12111 (2006)*

S. Blanco et al., *Ang. Chem. Int. Ed. (2016)*

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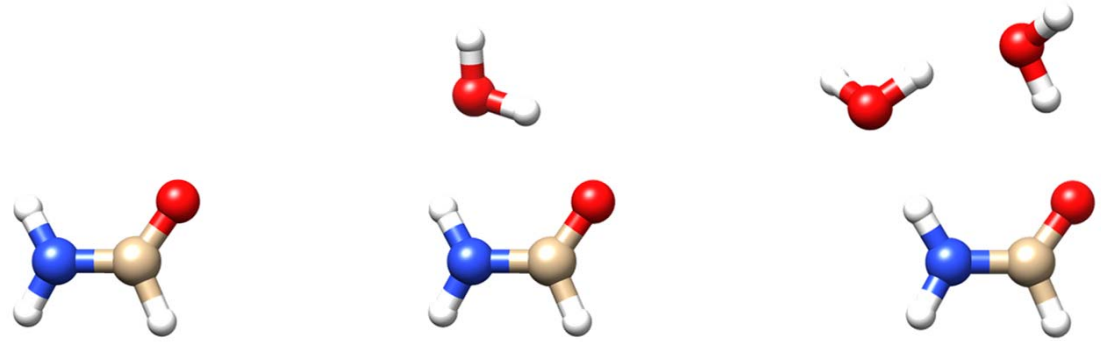

r_{C-N} = 1.361 Å

1.350 Å

1.343 Å

shortening of HB lengths

r(C-N) decrease

S. Blanco et al., *JACS* 128(37) *12111 (2006)*

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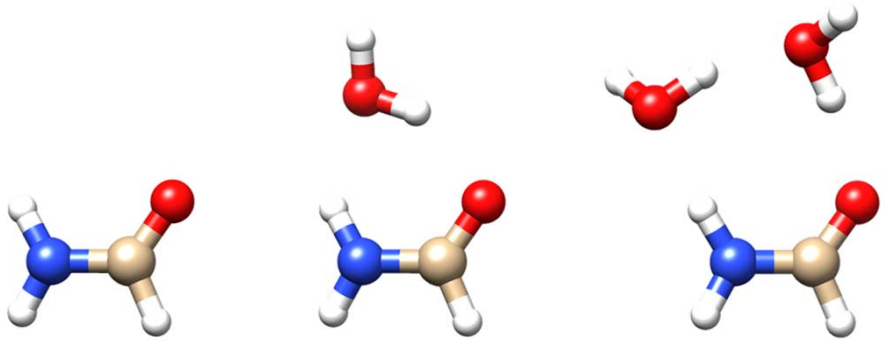

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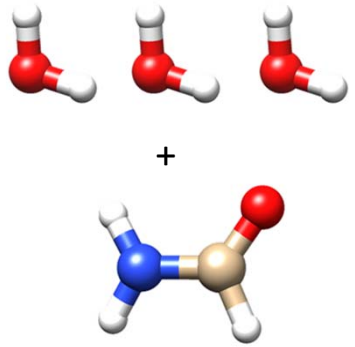

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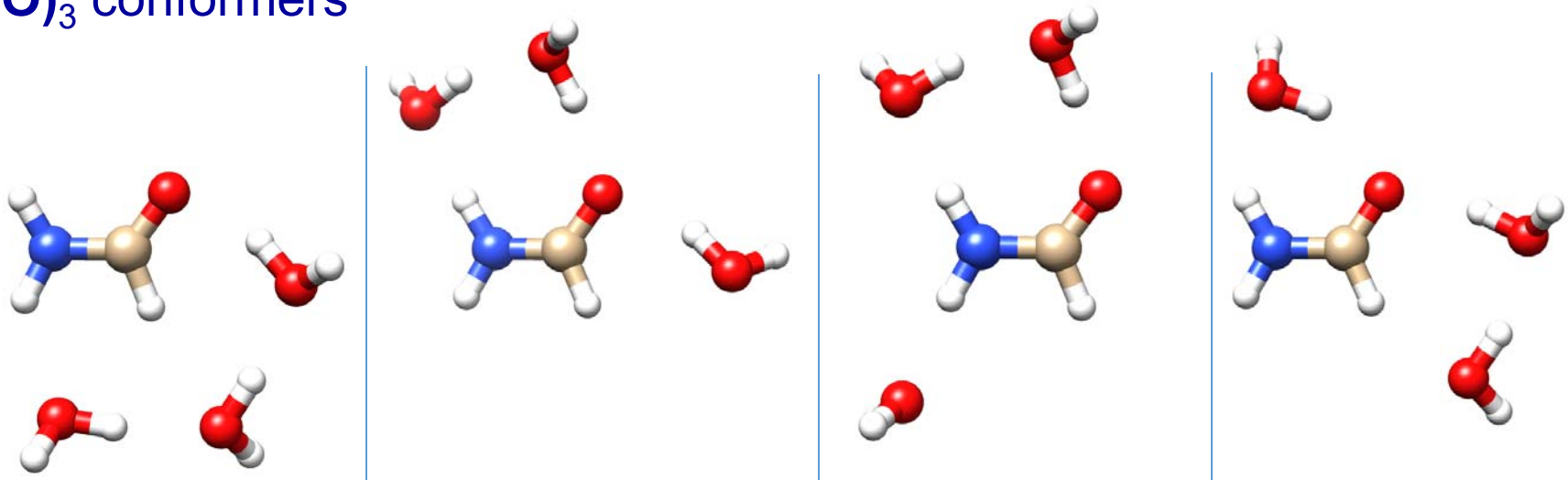
Formamide-$(H_2O)_3$ conformers

FW1+FW2



Parameter[(a)]	FW1-b ’b c	FW2a-FW1b	FW2a-FW1c	FW2b-FW1a
ΔE/ cm^{-1}				
ΔE/ $kJmol^{-1}$				
A/MHz				
B/MHz				
C/MHz				

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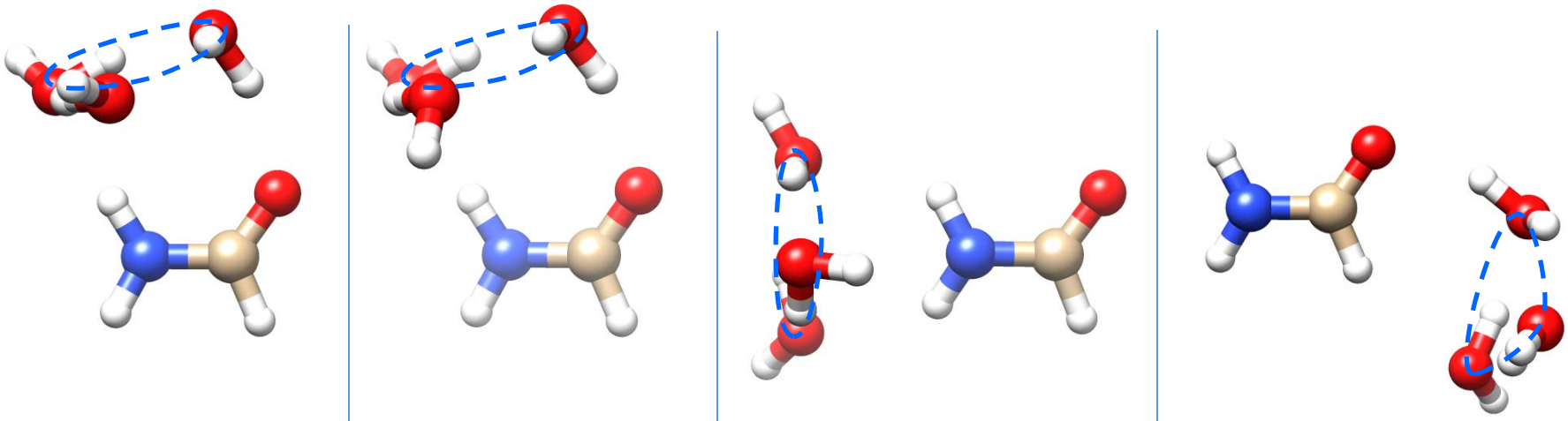
Formamide-$(H_2O)_3$ conformers

Cloud



Parameter[(a)]	C-top-u	C-top-d	C-back	C-front
ΔE/ cm^{-1}				
ΔE/ $kJmol^{-1}$				
A/MHz				
B/MHz				
C/MHz				

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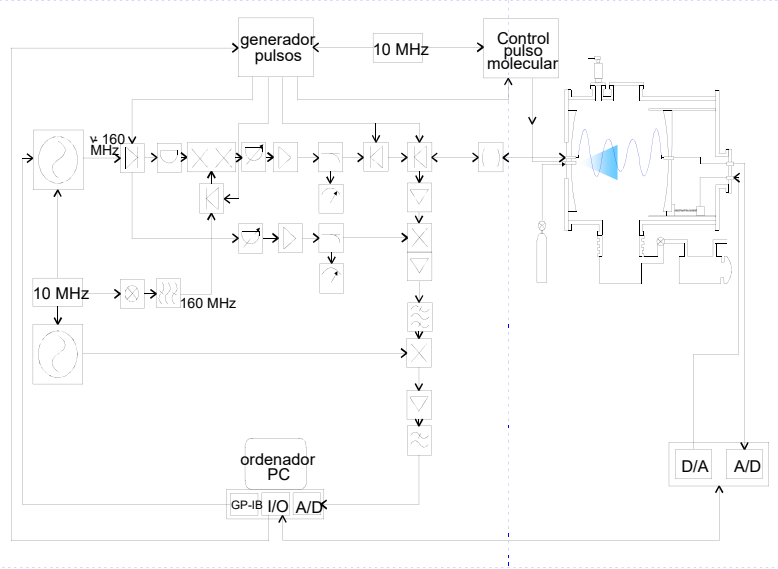
Spectrum



FTMW spectrometer

Fabry-Pérot cavity supersonic jet - sample

Chem. Phys. 218 267 (1997); Chem. Phys. 119 880 (2003)

MB-FTMW (4-16 GHz)

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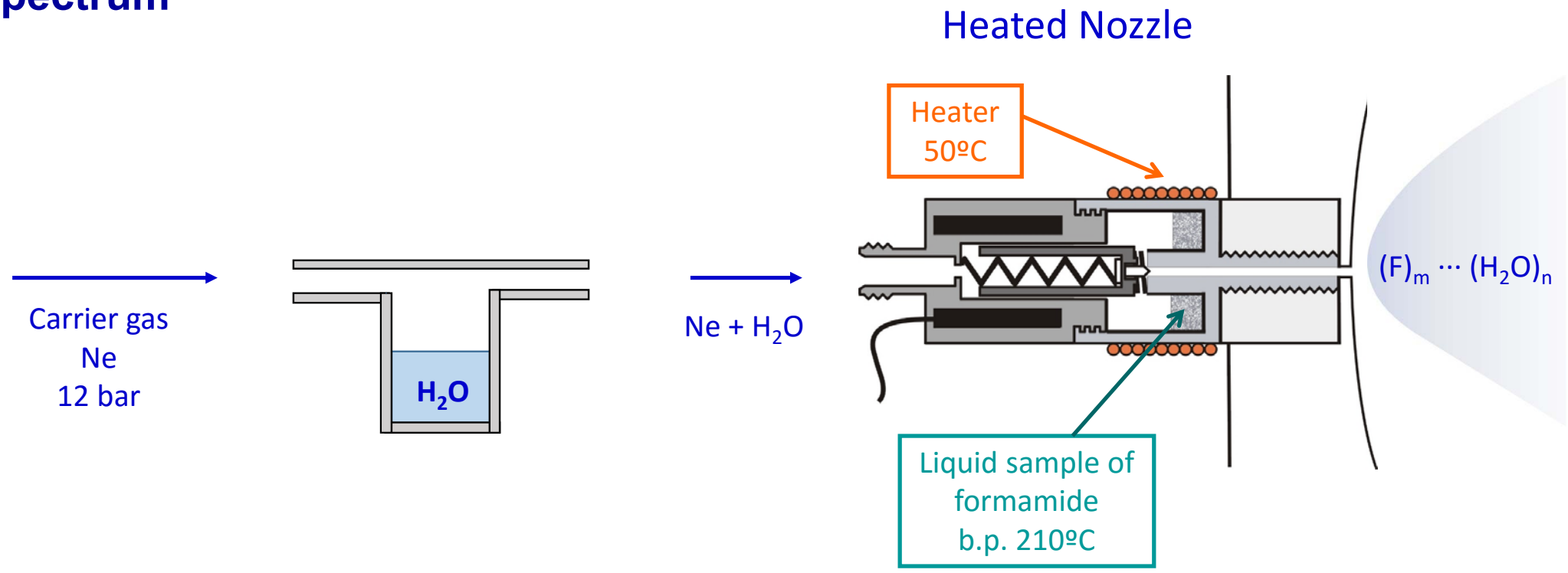
Spectrum



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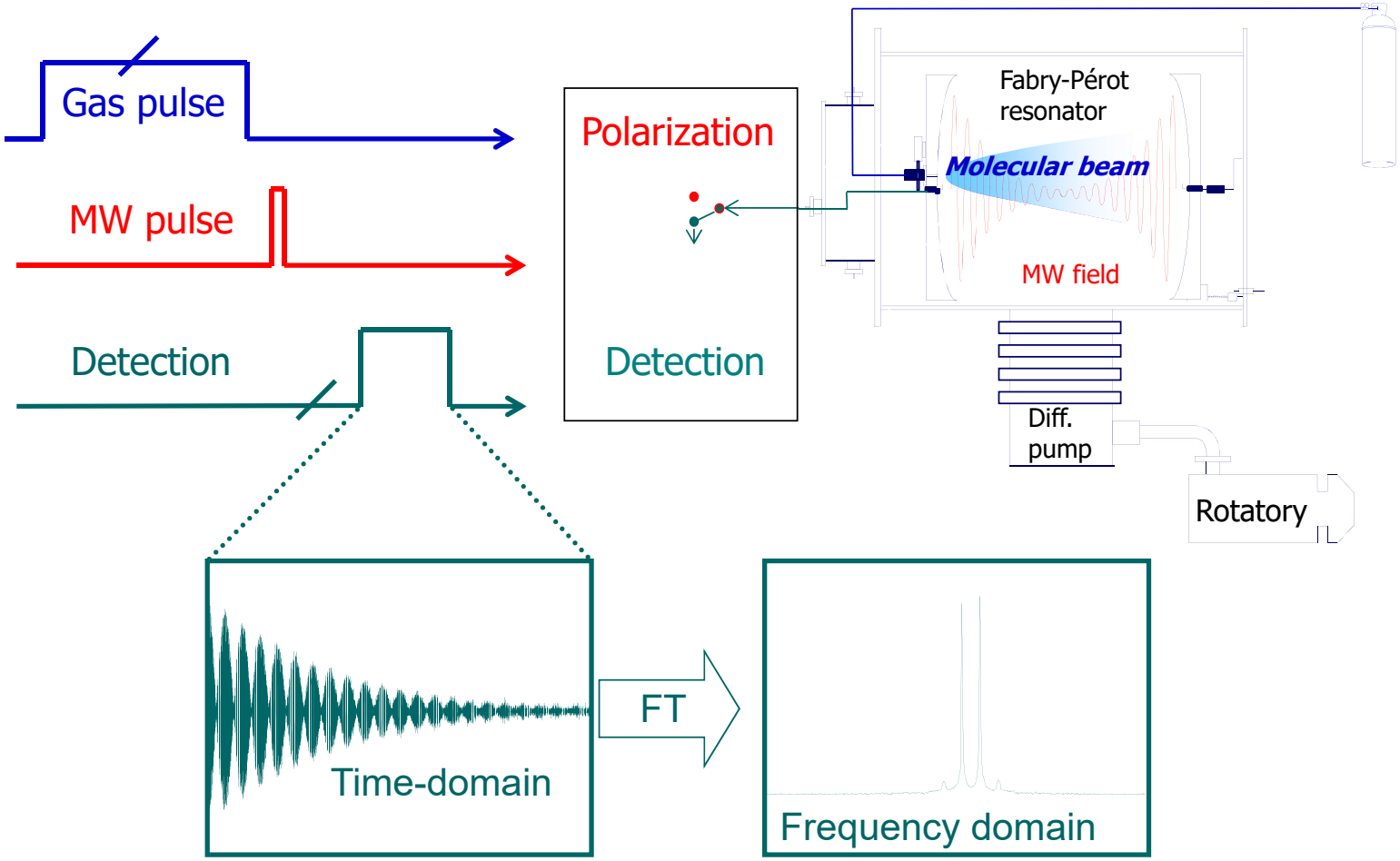
Spectrum



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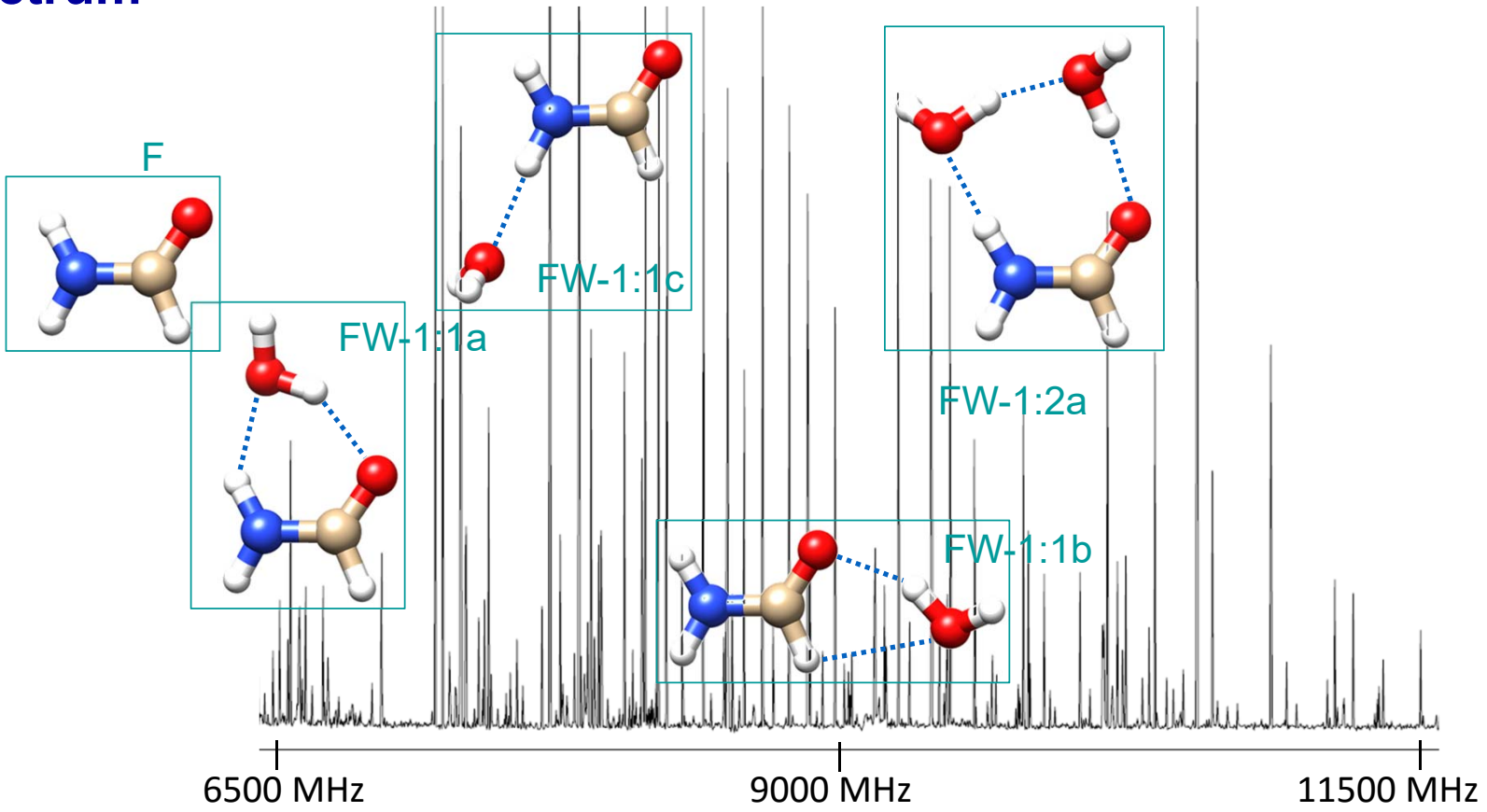

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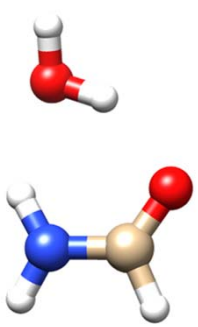
Evidences of cooperative effects such as **polarization enhanced** or **resonance assisted** hydrogen bonding.

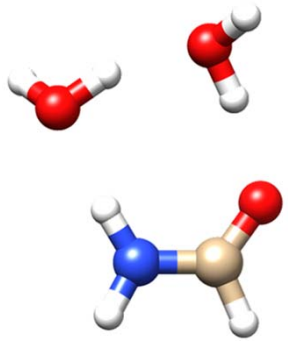


-

$r_{Hf\cdots Ow}$ = 2.062 Å
$r_{Hw\cdots Of}$ = 1.957 Å

-

$r_{Ow\cdots Of}$ = 2.813 Å



$r_{Hw\cdots Ow}$ = 1.791 Å
$r_{Hf\cdots Ow}$ = 1.886 Å / $r_{Hw\cdots Of}$ = 1.810 Å

$r_{Ow\cdots Ow}$ = 2.774 Å
$r_{Ow\cdots Of}$ = 2.728 Å

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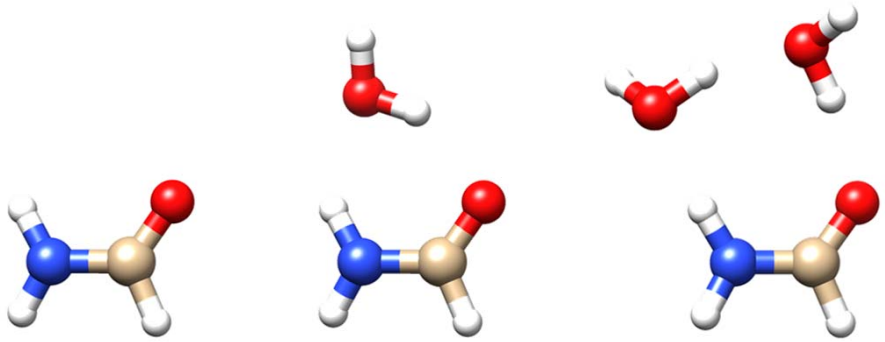

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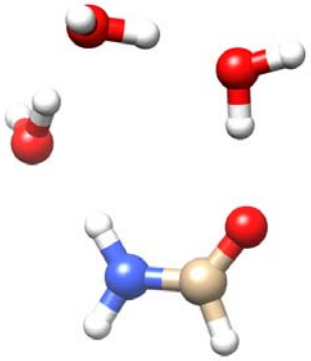

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